An Inequality Constrained Least-Squares Approach as an Alternative Estimation Procedure for Atmospheric Parameters from VLBI Observations

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Abstract On its way through the atmosphere, radio signals are delayed and affected by bending and attenuation effects relative to a theoretical path in vacuum. In particular, the neutral part of the atmosphere contributes considerably to the error budget of space-geodetic observations. At the same time, space-geodetic techniques become more and more important in the understanding of the Earth's atmosphere, because atmospheric parameters can be linked to the water vapor content in the atmosphere. The tropospheric delay is usually taken into account by applying an adequate model for the hydrostatic component and by additionally estimating zenith wet delays for the highly variable wet component. Sometimes, the Ordinary Least Squares (OLS) approach leads to negative estimates, which would be equivalent to negative water vapor in the atmosphere and does, of course, not reflect meteorological and physical conditions in a plausible way. To cope with this phenomenon, we introduce an Inequality Constrained Least Squares (ICLS) method from the field of convex optimization and use inequality constraints to force the tropospheric parameters to be non-negative allowing for a more realistic tropospheric parameter estimation in a meteorological sense. Because deficiencies in the a priori hydrostatic modeling are almost fully compensated by the tropospheric estimates, the ICLS approach urgently requires suitable a priori hydrostatic delays. In this paper, we briefly describe the ICLS method and validate its impact with regard to station positions.

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1 Introduction

Variable conditions in the neutral atmosphere contribute considerably to the error budget of space-geodetic techniques, such as Global Navigation Satellite Systems (GNSS) or Very Long Baseline Interferometry (VLBI). At the same time, space-geodetic observations play a steadily increasing role in the understanding of the Earth's atmosphere and become more and more important in interdisciplinary studies of climatology or meteorology. For instance, atmospheric parameters from Global Positioning System (GPS) observations are used for data assimilation procedures in global numerical weather models. VLBI observations are not used for these purposes, because the observations are not continuous and the global distribution and spatial coverage lags behind GPS observations. However, with regard to the VLBI Global Observing System (VGOS, [7]), the next generation VLBI system, which leads to an increasing number of observations as well as a better sky coverage and, therefore, a better sampling of the atmosphere, a more valuable contribution to atmospheric sciences could be possible, at least for calibration purposes.

On its way through the atmosphere, the signals of space-geodetic techniques are delayed and affected by bending and attenuation effects relative to a theoretical path in vacuum. The tropospheric delay is usually taken into account by applying an adequate model (e.g., the modified Saastamoinen formula [3]) for the hydrostatic component (index h) and by additionally estimating a correction parameter for the highly variable wet component (index w) within the VLBI parameter estimation process. Both components are modeled by a zenith delay (ΔL_h^z and ΔL_w^z) and a corresponding mapping function ($mf_h(\varepsilon)$ and $mf_w(\varepsilon)$) for the transformation from zenith to an arbitrary elevation angle ε. In addition, troposphere gradients in the North-South and East-West directions (G_{ns} and G_{ew}) can be estimated to overcome azimuthal asymmetries in the refractive index (second line of Equation 1, where α denotes the azimuth) [6],

$$\begin{aligned}\Delta L_t(\alpha,\varepsilon) = mf_h(\varepsilon)\Delta L_h^z + mf_w(\varepsilon)\Delta L_w^z \\ + mf_g(\varepsilon)\left[G_{ns}\cos(\alpha) + G_{ew}\sin(\alpha)\right].\end{aligned} \tag{1}$$

Unfortunately, the Ordinary Least Squares (OLS) approach sometimes leads to negative zenith wet delay (ZWD) estimates. Because ZWD parameters can be directly linked to the integrated water vapor content in the atmosphere, and there is of course nothing like negative water vapor, these atmospheric parameters obviously do not reflect meteorological and physical conditions in a plausible way. To overcome this issue, an Inequality Constrained Least Squares (ICLS) approach from the field of convex optimization [2] is introduced as an alternative estimation procedure for the determination of atmospheric parameters. Thus, the tropospheric parameters are constrained to non-negative values allowing for more realistic zenith wet delay estimates.

Special consideration should be given to the a priori hydrostatic delay, because mis-modeling a priori tropospheric data is compensated by the zenith wet delay estimates by almost 100%. If prohibited by inequality constraints, the erroneous hydrostatic delays can not be compensated by the ZWDs anymore, which then directly affects other correlated parameter groups such as the vertical component of the station positions. The influence of different inequality constraints for certain ZWD parameters and VLBI stations on the zenith wet delay estimates of the same station as well as on other parameter types is investigated in this study.

2 The Inequality Constrained Least Squares Method

The OLS model can be written as

$$\mathbf{l} = \mathbf{A}\mathbf{x} + \mathbf{v}, \tag{2}$$

$$\boldsymbol{\Sigma}_{ll} = \sigma_0\, \mathbf{Q}_{ll}, \tag{3}$$

where $\mathbf{l}$ denotes the vector of observations with corresponding variance-covariance matrix $\boldsymbol{\Sigma}_{ll}$ as the product of the a priori variance factor σ_0 and the cofactor matrix $\mathbf{Q}_{ll}$. The matrix $\mathbf{A}$ is the Jacobian matrix which contains the partial derivatives of the observation equations with respect to the parameters and $\mathbf{x}$ is the vector of unknown parameters to be estimated ($\tilde{\mathbf{x}}$ denotes the adjusted parameters). The vector

$$\mathbf{v} = \mathbf{A}\tilde{\mathbf{x}} - \mathbf{l} \tag{4}$$

contains the residuals. The optimal solution is obtained by minimizing the objective function, the (possibly weighted) square sum of residuals

$$\mathbf{v}^T \boldsymbol{\Sigma}_{ll}{}^{-1}\, \mathbf{v} \ldots \min. \tag{5}$$

In case of the ICLS method, the concept is extended by linear inequality constraints of the form

$$\mathbf{B}^{\mathbf{T}}\mathbf{x} \leq \mathbf{b}, \tag{6}$$

which have to be fulfilled strictly. Because it is not known in the beginning, which inequality constraints will become active and will influence the result, the ICLS problem can only be solved iteratively. In each iteration, the corresponding sets of active and inactive constraints change. In general, there are several iterative methods to solve such an ICLS problem. In this study, we made use of the so-called Active Set method [4], a simplex algorithm, which follows the boundary of the feasible set, i.e., the region where all inequality constraints are fulfilled, until the optimal solution is reached. For more details, see [5] or [10].

Due to the missing analytic relationship between observations and parameters, the calculation of standard deviations in the Least Squares sense is not possible anymore. Thus, to allow for a suitable quality description of the derived parameters, we make use of Monte Carlo simulations to obtain a discrete approximation of the probability density function. Instead of standard deviations, so-called highest probability density intervals are calculated to overcome asymmetric probability density functions caused by inequality constraints [9].

3 Results

In order to validate the ICLS method, we make use of about 125 VLBI sessions provided by the International VLBI Service for Geodesy and Astrometry (IVS, [11], [8]). The databases are processed using the VLBI data analysis software ivg::ASCOT [1], which is being developed by the VLBI group of the Institute of Geodesy and Geoinformation of the University of Bonn. The modeling and analysis setup described in [5] is used for all solutions.

In Figure 1, the zenith wet delay estimates are exemplarily illustrated for the VLBI station GILCREEK (Gilmore Creek, Alaska) and a VLBI session on November 28, 2001. The ZWD parameters derived from the Least Squares solution are represented as black triangles while the ICLS estimates are depicted as gray circles. The second OLS parameter, for instance, is negative by about 3 mm and is shifted to a non-negative value in the ICLS approach. Because continuous piece-wise linear functions are used for the parametrization of the atmospheric parameters, all zenith wet delay estimates of the same VLBI station are correlated and, as a consequence, many of the ZWDs shown in Figure 1 are also shifted. However, the ZWD differences between the OLS and ICLS solution are not significant, except for the parameter where the inequality constraint is active. This holds for the general case as well.

Even more interesting is the influence of this single inequality constraint (applied for one atmospheric parameter) on other parameter groups, especially because different parameter types, such as clock parameters, zenith wet delays, and the vertical component of the stations positions, are correlated within the VLBI parameter estimation procedure. This effect is shown in Figure 2.

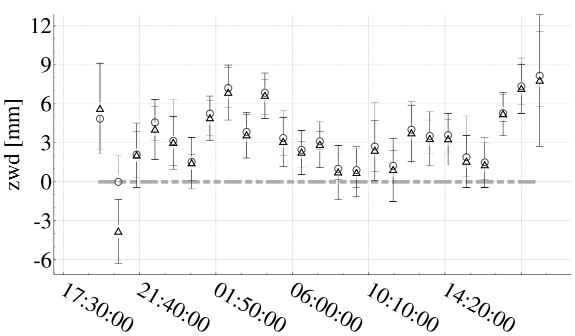
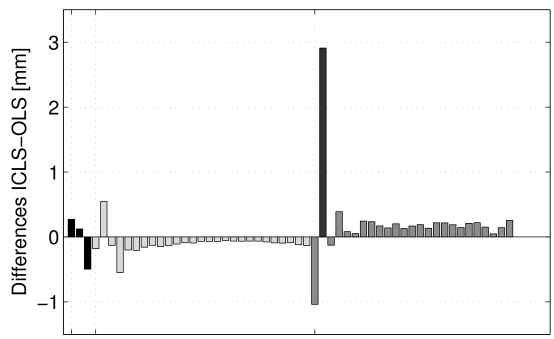
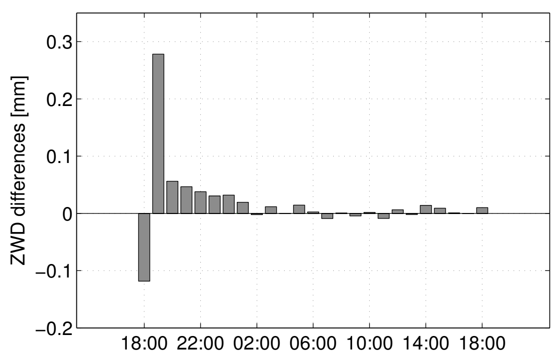


Fig. 1 Zenith wet delay parameters for the VLBI station GILCREEK (Gilmore Creek, Alaska) on November 28, 2001. The Least Squares estimates are represented as black triangles and the Inequality Constrained Least Squares solution is depicted as gray circles.



(a)



(b)

Fig. 2 (a) The influence of a single ZWD inequality constraint (dimmed gray) on station coordinates (black), clocks (light gray), and zenith wet delays (dark gray) of the same station (Gilmore Creek, Alaska). (b) The influence of the same inequality constraint on zenith wet delay parameters (dark gray) of another station (Matera, Italy).

The influence of a single inequality constraint applied to only one zenith wet delay of the station GILCREEK (dimmed gray) on the station coordinates (black), the clock model correction parameters (light gray), and the zenith wet delays (dark gray) of the same station is depicted in Figure 2(a). Here, it becomes obvious that less than one millimeter of the difference between the ICLS and OLS solution of approximately 3 mm is compensated by the vertical component of the telescope coordinates. The maximum difference can be

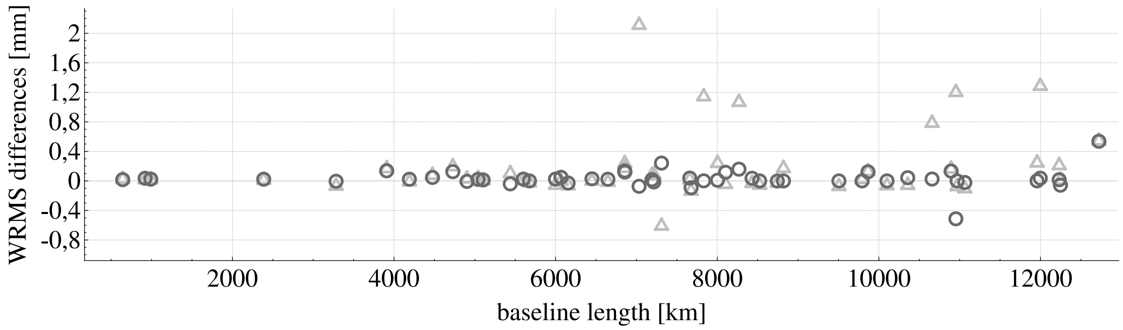


Fig. 3 Baseline length repeatability differences with respect to the OLS solution. The light gray triangles represent an ICLS solution, where the meteorological data used for the calculation of the hydrostatic delay only results from in-situ measurements, while dark gray circles depict an ICLS solution using atmospheric a priori data derived from a combination of in-situ observations and a numerical weather model of the ECMWF.

found in one of the ZWD estimates (about 1 mm). The remaining part is evenly distributed between the other parameters, although the differences are on the order of tenths of a millimeter and of course not significant. Figure 2(b) shows the influence of the same inequality constraint on the zenith wet delay estimates of another station, here exemplarily for MATERA (Matera, Italy). The differences between both solutions are again on the order of tenths of a millimeter, which indicates that the use of the ICLS method only leads to an effect on estimates of the same station for which inequality constraints are applied.

In the following, particularly the effect of inequality constraints on station coordinates will be investigated in more detail. Thus, the differences in baseline length repeatabilities between the Least Squares and the ICLS method are calculated for 125 VLBI sessions in 2002. For about 20% of these sessions automatically inequality constraints are applied for at least one station and one zenith wet delay parameter. The results are depicted in Figure 3, where the baseline length repeatability differences of two ICLS realizations with respect to the Least Squares solution are represented by light gray triangles and dark gray circles, respectively. Both ICLS solutions only differ in the meteorological data (i.e., temperature and pressure) used for the modified Saastamoinen formula [3]. In the first solution, meteorological data from in-situ measurements as observed at the VLBI sites are applied (light gray triangles). However, these data may contain data gaps and outliers. As a consequence, mis-modeling in the a priori data occurs, which is compensated by the zenith wet delay estimates by almost 100%. When introducing inequality constraints, this compensation effect is suppressed and affects other correlated parameter groups like the vertical component of the telescope positions. This then leads to a degradation of the baseline length repeatabilities (light gray triangles). Thus, special attention has to be paid to the a priori modeling of the zenith hydrostatic delays.

In the second solution (dark gray circles) a numerical weather model of the European Center for Medium Weather Forecast (ECMWF) is used to define the level of the meteorological data, while their variability is taken from the in-situ observations after removing outliers and filling data gaps. As a consequence, the differences between this realization and the OLS solution are not significant anymore, although inequality constraints are introduced to allow for a more reliable estimation of tropospheric parameters.

Please note that approximately the same number of inequality constraints is needed for both ICLS realizations, although the constrained parameters can be different and the order of magnitude in the differences between the ICLS and OLS can vary. Thus, it has to be concluded that the negative zenith wet delay estimates result not only from a priori mis-modeling. In fact, there are several other "dirt" effects on the ZWD parameters, such as mis-modeling of geophysical effects as well as certain impact due to instrumental delays or the clock parametrization. This has to be investigated in more detail in the future. In addition, the tropospheric parameters in cold regions derived alternatively have to be validated with regard to numerical weather models or other space-geodetic techniques like GPS or GNSS in general.

4 Conclusion and Future Work

Sometimes, the OLS method leads to negative zenith wet delay parameters. In a meteorological sense, that would be equivalent to negative water vapor in the atmosphere. In order to constrain these parameters to non-negative estimates and, therefore, to allow for more realistic tropospheric parameters, an ICLS approach is introduced. The influence of inequality constraints on zenith wet delay parameters as well as on other parameter groups has been investigated leading to the following results. The use of the ICLS method solely affects parameters of the same station, where inequality constraints are active. The differences between the ICLS and OLS solutions due to the inequality constraints are partly compensated by the vertical component of the station coordinates. However, the differences in baseline length repeatabilities between both solutions are not significant if the a priori hydrostatic model is not affected by outliers, data gaps, or mis-modeling issues. Thus, the use of inequality constraints is, in principle, possible without disturbing the VLBI target parameters. However, further investigations need to be carried out concerning other "dirt" effects compensated by the ZWD parameters. Additionally, an external validation for the newly derived tropospheric parameters is necessary, which can be achieved using either numerical weather models or ZWD time series from GPS observations.

Due to the discontinuous nature of VLBI observations, the tropospheric parameters can, of course, not yet be used for atmospheric purposes in terms of a data assimilation process. However, zenith wet delay estimates could, in fact, act as calibration parameters for numerical models or other space-geodetic techniques, at least as soon as a better coverage of the atmosphere becomes reality within the scope of VGOS networks.

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